UCID- 20297-85-3

LAWRENCE LIVERMORE NATIONAL LABORATORY
GRANULAR FLOW PROJECT - QUARTERLY REPORT

July - September 1985

Edited by
O. R. Walton

For
U.S. Department of Energy
Office of Fossil Energy
Pittsburgh Energy Technology Center
Pittsburgh, Pennsylvania

September 30, 1985

Lawrence
Livermore
National
Laboratory

Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161
Price: Printed Copy $ Microfiche $4.50

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During FY85 LLNL's Granular Flow Project has been primarily concerned with developing new discrete particle computer models for simulating the flow behavior of granular solids and determining their rheological characteristics. Calculations of effective viscosity, granular-temperature and stresses performed with our new two-dimensional steady-state shearing model for inelastic, frictional disks have been reported previously [1,2]. During the current reporting period most of our efforts have been directed toward completing an initial version of a three-dimensional model capable of doing similar calculations for assemblies of inelastic spheres. Some aspects of this model development effort were very straight forward extensions of our two-dimensional model, while others required significant new development effort.

In addition to getting the new three-dimensional model up and running on the CDC7600 computers during this reporting period we also:

- wrote algorithms to integrate the orientation coordinates of the particles in terms of quaternion parameters (a technique more efficient and accurate than using Euler angles),
- wrote a new algorithm for generating the initial packing of particles in the calculational cell,
- conducted preliminary tests of the integration equations, shearing algorithms and diagnostic calculations in our new model by comparing the results of this model with those of existing molecular dynamics models,
- started development of a new post processing program for the three-dimensional model including pictures of the particle positions and orientations,
- finalized algorithms for the frictional forces acting between spheres, and

- o started making measurements of stiffness and friction properties of the plastic disks used in air-table experiments at Clarkson University.

3-D Shear Model -- Inelastic Spheres

The 2DSHEAR model was extended to three dimensions. This new three-dimensional steady-state shearing model calculates the motion of spheres in a rectangular primary cell surrounded on all sides by periodic images of the primary cell. The image cells above and below the primary cell move at constant velocity to the right and left, respectively. Shearing is constrained to the x-direction in planes perpendicular to the y-axis. The model calculates the translational and rotational coordinates and velocities for each particle in the primary cell as a function of time. In addition, many other diagnostic quantities are calculated at specified time intervals for the entire cell as well as for two-dimensional zones perpendicular to the y-axis. These diagnostics include: r.m.s. velocity (deviatoric), mean x-velocity (total), spin angular momenta (x, y, and z), strain rate, packing density, translational kinetic energy density, translational potential energy density, rotational kinetic energy density, compressibility, viscosity, ratio of shear velocity to deviatoric velocity, and the kinetic and potential contributions to the stress tensor.

Four different normal force options are available in the model. They are: 1) a 12th power potential repulsive force (molecular force model), 2) a 3/2 power (of relative overlap) repulsive Hertzian contact force for perfectly elastic spheres, 3) a partially latching, or 4) a variable-latching spring model for inelastic spheres (analogous to the models reported previously [1,2]). Frictional forces have not yet been incorporated into the 3DSHEAR model. In order to maintain steady-state conditions with energy constantly being fed into the system due to the forced shearing, a "constant temperature" algorithm that scales the velocities of all particles on every time step to maintain a constant deviatoric kinetic energy in the cell is usually employed when one of the perfectly elastic (energy conserving) force models is used. The constant temperature algorithm is not needed when inelastic collisions are used since the system determines its own "natural" granular temperature.

Quaternion Parameters

Forces from all near-neighbor particles are accumulated for each particle on each time step and a second-order, explicit, integration algorithm (leap-frog technique) is used to determine the trajectories of each particle in the system. For particles with spherical symmetry the angular orientation of the particle itself is not needed to determine the changes in the rotational velocity. We only need to know the orientation and magnitude of the current rotational velocity of each particle and the (vector) torque acting on it. However, in order to display the current orientations of the spheres in computer movies we do need to have orientation information. For this reason and because we will eventually be concerned with non-symmeteric particles, we developed algorithms to calculate four quaternion parameters representating the orientation of each sphere. Only three of these parameters are independent with a normalization condition supplying the necessary forth equation for closure. We use a set of four first-order finite-difference equations to incrementally integrate the quaternion parameters (with the change in each quaternion determined by the mid-time-step rotational velocity components). We then apply the normalization condition uniformly to each of the four quaternions for each particle on each time step. The elements of the current rotation matrix giving the orientation of a given sphere are obtained from simple products and sums of the four quaternions [3]. To test the accuracy of this quaternion integration technique we ran test calcualtions for a particle freely spinning about an arbitrary axis in space and compared the accuracy of the subsequent orientations calculated by the quaternion method with those calculated by successive application of incremental orthogonal rotations on each time step. We repeated these calculations for various ratios of time step to angular speed and in every case the quaternion method was significantly more accurate and took a comparable amount of computer time.

Initial Packing and Time Averages

In the 2DSHEAR model the center of each particle was located at lattice points of an expanded hexagonal crystalline array, before shearing was started. An extension of this initialization procedure to three dimensions would be adequate for systems containing spheres of equal size; however, at high solids packings with a distribution of sizes, significant overlap of particles could result. In order to handle wide size distributions at any realistic solids packing we wrote a new initialization algorithm. In the new algorithm a set of initial particle center coordinates are randomly located throughout the primary cell. A temporary initial radius for each particle is chosen to be the largest possible value without exceeding the final desired radius or overlapping any other particle. A special initialization calculation is then performed during which the particles not already at their final size are gradually expanded while the calculated interparticulate forces cause any particles that begin to interpenetrate to move apart. During this initialization the velocities are set to zero on each time step (i.e. inertia is ignored) and the rate of expansion and the time step for this procedure are choosen so that the forces caused by the expansion of two contacting particles during one time step will move them apart further than the increment of expansion unless they are constrained by contacting more than one particle. We have tested this algorithm over a range of solids packings from 0.5 to

0.8. The resulting potential energy in the final (initialized) configuration (due to remaining contact forces) increased smoothly and monotonically over this range, even for packing fractions that exceeded the close-packed fraction of 0.74.

When shearing is started after the initialization calculation we find significant relaxation of the contact forces with some particles moving at relatively high velocities for a short period of time. This anomolous behavior quickly damps out as steady-state shearing is established. Our cumulative time averages of all quantities of interest are restarted once steady-state is achieved. Time history plots of various quantities verify that steady-state is indeed attained before the restart time. Figure 1 shows the cumulative time average r.m.s. deviatoric velocity as a function of time for a calculation with 125 particles having a coefficient of restitution of 0.8 and shearing at a strain rate of 5 inverse time units. In this calculation the cumulative time average was restarted at time, t=1.0, after steady-state had been achieved. The cumulative average plot (solid line) shows a discontinuity when the accumulation was restarted. The dashed line on the plot is a series of cumulative time averages over each of 400 small time intervals (each with approximately 225 calculational time steps). This plot of the short time interval averages indicates that steady-state was probably attained at a time as early as 0.25 for this calculation. The entire calculation took nearly an hour of CDC7600 computer time.

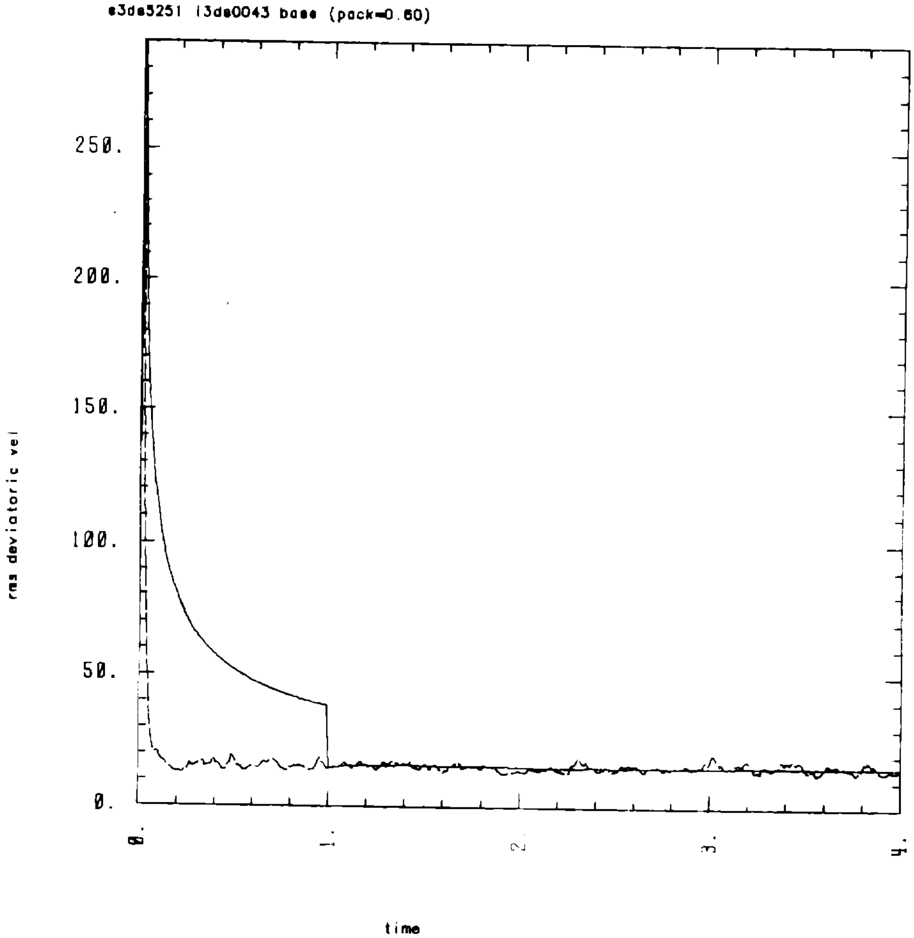

Figure 1. Cumulative time averages of the r.m.s. deviatoric velocity in a steady shearing calcualtion with 125 particles, e = 0.8, $\nu = 0.6$, $\dot{\epsilon} = 5$.

<u>Verification Calculations</u>

As a test of the accuracy of the integration scheme, the correctness of the cumulative time averaging algorithms for the nine components of the stress tensor and the overall validity of our three-dimensional steady state shearing algorithms, we compared the results of our new model with Hoover's molecular dynamics calculations of the stress tensor for soft spheres in plane couette flow[4]. Using a 12th-power pair potential $\phi = \epsilon(\sigma/r)^{12}$ with ϵ, σ and the particle mass, m, all set to 1.00, a 256 particle system with a constant kinetic energy of 1.465 per particle was calculated at a shear rate of one and at a solid packing of $\nu = 0.444288$ which corresponds to Hoover's reduced density, ν/ν_{max} of 0.600. The calculation was run for a total time of 100 using a time step of $\Delta t = 0.005988$. The parameters correspond to those of Hoover except his calculation was run to a final time of 500. The resulting mean total energy per particle was 3.654 compared to 3.656 for Hoover's calculation. The resulting kinetic and potential contributions to the total stress tensor are given in Table 1. The numbers in parenthesis are the deviation from Hoover's values. His stated uncertainties were "of order 0.002" in the kinetic part and "of order 0.005" in the potential part. As can be seen from Table 1 the values we obtained for the components of the stress tensor are quite close to those obtained by Hoover. The largest deviations appear in the potential contributions, yet the trace of the stress tensor we calculate is within 0.005 of the value obtained by Hoover. We did not run our calculation further to establish uncertainties in our calculated values; but, based on the values obtained, concluded that the basic integration and diagnostic algorithms in our model are essentially working properly. (It should be noted that we truncated the interparticulate force at a center-to-center separation of 2.458. Hoover did not specify if a truncation distance was used in his calculations).

TABLE 1.
Stress tensor for 256 particles in steady shear (12th power potential)

Kinetic contributions to the stress tensor

0.844 (-0.004)	-0.104 (+0.001)	0.000 (0)
-0.104 (+0.001)	0.829 (+0.002)	0.000 (0)
0.000 (0)	0.000 (0)	0.813 (+0.001)

Potential contributions to the stress tensor

7.419 (-0.024)	-1.106 (+0.019)	0.002 (+0.002)
-1.106 (+0.019)	7.499 (-0.003)	-0.013 (-0.013)
0.002 (+0.002)	-0.013 (-0.013)	7.377 (+0.022)

Steady-State Shearing with Inelastic Spheres

Calculations of steady-state shearing with inelastic spheres are in progress. Preliminary results for a calculation with 125 particles with a coefficient of restitution, e = 0.8, shearing at a rate of ε = 5.0, at a solids packing fraction ν = 0.50, are within about ten percent of the theoretical predictions for the same case by Lun et al. [5] as shown in Table 2.

TABLE 2.

Preliminary results for 125 particles with e = 0.8, ν = 0.5, $\dot{\varepsilon}$ = 5.

Quantity	Present calculation	Theory [5]
$R = (\sigma \lvert du_x/dy \rvert / \langle v^2 \rangle^{1/2}$	0.92	0.88
Normal Stress P_{yy}	68.5	59.7 (1.0)*
Shear Stress P_{xy}	25.9	23.9 (2.5)*
P_{xy}/P_{yy}	0.38	0.40

*Numbers in parenthesis are the reduced values reported by Lunn et al.. They have been multiplied by a factor of $75/\pi$ to convert to the units in our calculations.

Another calculation at a solids packing ν = 0.60 is producing stresses that are significantly higher than the Lun et al. theory. It is too early to determine conclusively the reason for the differences at this higher solids packing, but it may be due to the effects of enduring contacts at high concentrations. These effects are not included in the theory of Lun et al.

Post Processing 3-D Model

A new post processing graphics routine has been written to plot the results of various diagnostic calculations from the new three-dimensional steady-state shearing model. This graphics package can be used to make time-history plots of any of approximately 30 different quantities, translational and angular velocity-distribution plots and zonal plots showing the variation of various quantities from the top to the bottom of the cell. Particle positions and orientations are plotted as either orthographic or perspective projections onto any specified view plane. The orientations of the particles are indicated by the location of three great circles initially corresponding with the intersections of planes perpendicular to the x, y, and z-axes passing through the spheres' centers. The great circles move subsequently with the spheres as they rotate in response to tangential forces. Figure 2 shows an orthographic projection of 216 particles in the primary calculational cell during a steady-shearing calculation with 12th-power potential forces acting between particles (no friction and thus no rotations were present in this calculation). Further work is underway to include fractional periodic image particles on the edges of the cell and more than one cell in the orthographic and perspective projections.

Friction Force Model

A two-dimensional friction force model (for forces acting between three dimensional objects) has been adapted for contacts between two spheres. The model incrementally increases the frictional resistance to tangential displacements until full sliding occurs. The stiffness for each incremental change in friction force depends on the current force value and the direction of the slip. For contacts between bodies with curved surfaces the tangent-plane at the point of contact can change as the positions of the particles change. In order to facilitate vector addition of various terms contributing to the slip displacement during a single time step, all vectors associated with the tangential friction force are projected or rotated into the current tangent plane. The effects of the incremental slip displacement on the current tangential friction force are then determined and a new friction force to be applied during the next time step is calculated. For motions restricted to a single plane this new model generates forces that are the same as those used in our previous two-dimensional disk model. We plan to incorporate this model into the 3DSHEAR program during the next reporting period.

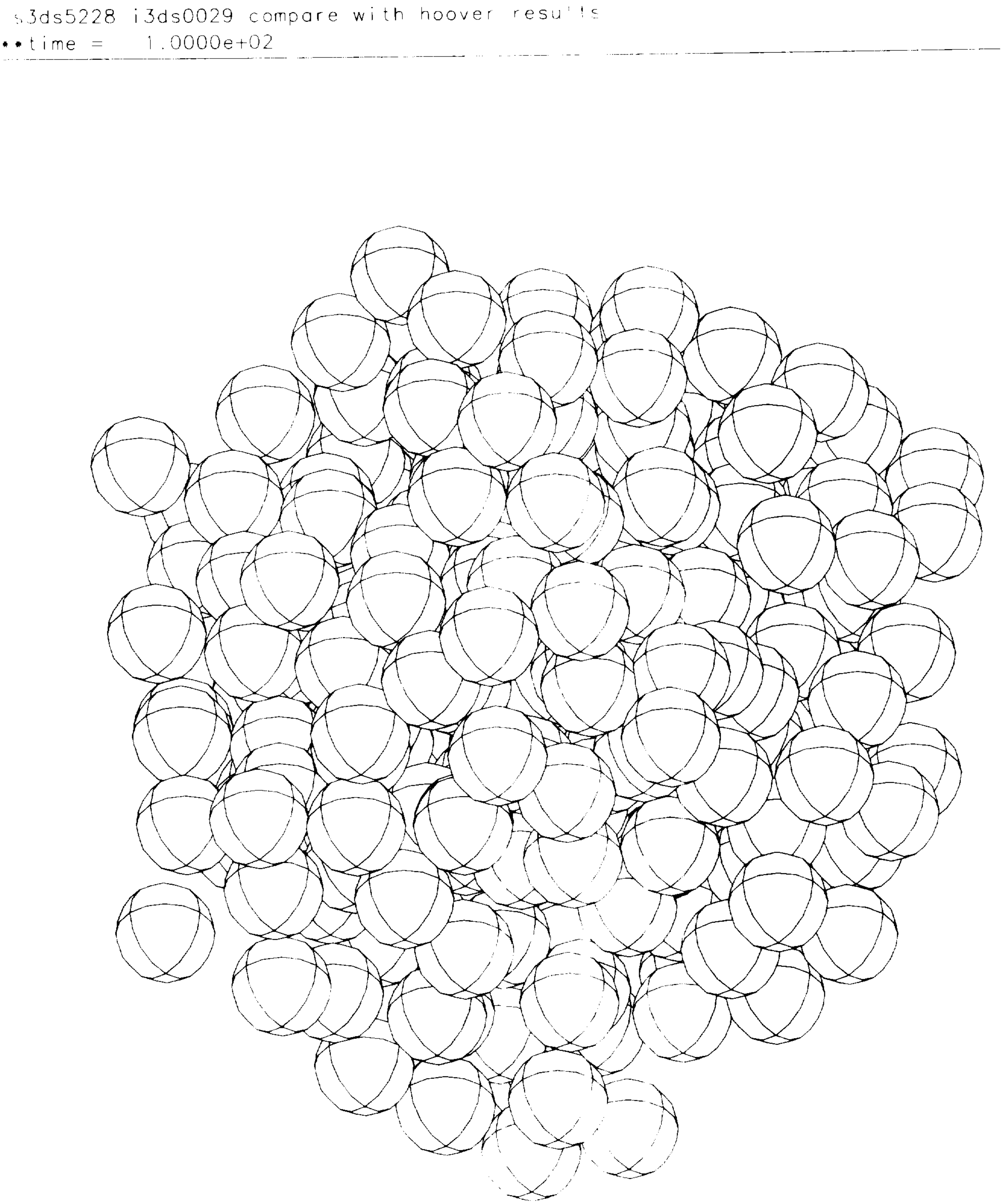

Figure 2. Orthographic projection of 216 spheres in primary calculational cell of steady shearing calculation using 12th power potential forces.

Physical Tests of Plastic Disks

We have requested and obtained several plastic disks from Professors Ackerman and Shen at Clarkson University. These are the same disks as are being used in air-table tests of shearing flows in two-dimensions. We have begun a set of measurements to determine the normal and shear stiffnesses of the disks and the effective friction coefficients for edge-on contacts. Preliminary results on the normal force measurements indicate that the material is highly rate sensitive. We anticipate obtaining coefficient of restitution vs. impact velocity information from Clarkson University in the near future. Once our stiffness and friction tests are completed and we have the restitution data from Clarkson, we will determine appropriate values for our force model parameters so we can simulate the air-table flow tests.

Presentations & Publications

O.R. Walton,"Granular Flow: AR&TD Contract Rewiew", Presented at DOE, Fossil Energy AR&TD Direct Utilization Contractors Mtg., 13-15 Aug. 1985, Morgantown, WV, (also: UCRL-92992 preprint, July 19, 1985).

O.R. Walton, "Rheology of Assemblies of Inelastic, Frictional Particles", Microgravity Particle Research Facility Workshop, NASA - Ames Research Center, 22-24 Aug 1985, Moffett Field, CA.

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2. Granluar Flow Project - Quarterly Reports, edited by O.R. Walton, Lawrence Livermore National Laboratory Reports UCID-20297-84-4 through 85-2.

3. D.J. Evans, "On the representation of orientation space", Molec. Physics, 1977, Vol. 34, No. 2, 317-325. and also: D.J.Evans and S. Murad, "Singularity free algorithm for molecular dynamics simulation of rigid polyatomics", Molec. Physics, 1977, Vol. 34, p327.

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